REMOTE SENSING OF TEMPERATURE BY THE STRATOSPHERIC AEROSOL AND GAS EXPERIMENT III

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Abstract

The Stratospheric Aerosol and Gas Experiment III (SAGE III) will use solar and lunar occultation measurements of atmospheric transmission to retrieve vertical profiles of O_3, NO_2, H_2O, NO_3, OClO, aerosol extinction, temperature, and pressure. Remote sensing of temperature and pressure will be performed utilizing multiwavelength measurements of the oxygen A-band absorption spectra in the visible wavelength region between 759 and 771 nm. Details of the retrieval algorithm are presented and results of simulated retrievals are shown to illustrate the feasibility of the approach.

1. Introduction

The Stratospheric Aerosol and Gas Experiment III (SAGE III) is part of NASA's Mission to Planet Earth (MTPE) Earth Observing System (EOS) program. SAGE III will provide limb occulation measurements of multiwavelength aerosol extinction (8 wavelengths) and vertical profiles of ozone, nitrogen dioxide, water vapor, temperature, and pressure. A lunar occultation capability permits the additional retrieval of nitrogen trioxide and chlorine dioxide. The first flight of SAGE III will be on the Russian Space Agency's METEOR 3M-1 spacecraft in August 1998 in a high-inclination orbit with additional deployments scheduled on the International Space Station (~2002) in a mid-inclination orbit and on a flight of opportunity (FOO) mission (~2005) in a high-inclination orbit.

Remote sensing of temperature and pressure will be performed using SAGE III measurements of the oxygen A-band absorption spectra centered near 760 nm. Temperature and pressure measurements are essential to SAGE III for computing both Rayleigh scattering and atmospheric refraction and retrieving mass mixing ratios of gaseous species on pressure surfaces. The addition of a temperature and pressure retrieval capability to SAGE III will eliminate the need for an external source of these data. In addition, an accurate determination of the vertical distribution of temperature by SAGE III will provide a unique self-calibrated, high vertical resolution data set for monitoring temperature changes in the stratosphere and mesosphere.

An overview of the SAGE III temperature and pressure retrieval process is presented below. Results from simulated retrievals are used to illustrate the feasibility of the approach. Uncertainties involved with the retrieval algorithm will also be discussed.

2. SAGE III Measurements

SAGE III is the fifth generation of solar occultation instruments designed to measure atmospheric aerosols and gaseous species. The concept began as a simple hand-held, one channel, manually operated sunphotometer, but with each generation of evolution, the instrument became more complex in design and possessed additional measurement capabilities (see e.g., Pepin et al. 1976; McCormick et al., 1979; Mauldin, 1984). The current SAGE III design utilizes an 800 element CCD linear array detector to provide spectral coverage from 280 to 1030 nm, together with a single photodiode detector at 1550 nm which was added to improve sensitivity to large aerosol particles (McCormick et al., 1991). The incorporation of the CCD array will permit the measurement of gaseous species from the multichannel absorption signatures simplifying the retrieval process and 16-bit digitization will improve the precision and altitude range of the measurements.

The oxygen A-band possesses several features which make it well-suited for remote temperature sensing. The line strengths at the center of the absorption band are quite strong; therefore, high signal-to-noise measurements can be obtained near the band center. In addition, the temperature dependence of the line strengths varies from positive to negative over the A-band spectra. For example, at wavelengths far away from the band center, the line strengths decrease with increasing temperature, while at wavelengths close to the band center, the line strengths decrease with increasing temperature. These unique sensitivities of the line strengths to temperature can be utilized for accurate temperature profile sensing.

SAGE III will make measurements across the oxygen A-band from approximately 759 to 771 nm with a resolution of about 1.4 nm. The spectra will be oversampled with 14 channels equally spaced at intervals of approximately 1 nm. Figure 1 illustrates both the fine structure present in the oxygen A-band absorption spectrum and the spectral resolution attainable with SAGE III. In addition to molecular oxygen, Rayleigh scattering, aerosol, and ozone also contribute to the extinction over the A-band spectral region and must be removed from the measured slant path optical depth before performing the inversion. The Rayleigh contribution will be estimated using temperature and pressure profiles provided by the NASA Goddard Space Flight Center's Data Assimilation Office (DAO). The aerosol correction will be estimated from aerosol measurements at 757 and 872 nm. The ozone correction is a straight forward product of the multiple linear regression technique used to retrieve ozone profiles. Once the contributions for these additional species are removed from the total A-band slant path absorption, the residual oxygen slant path absorptivities will be inverted to produce profiles of temperature and pressure.

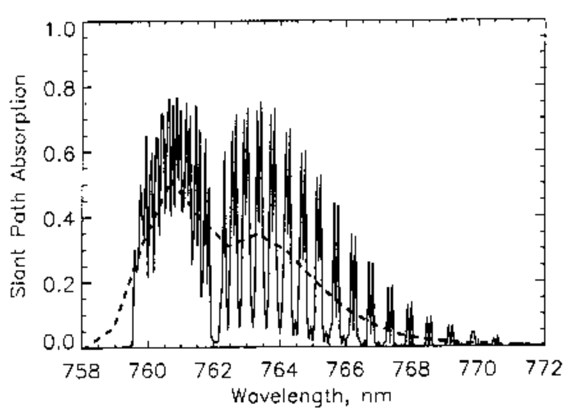

Figure 1. Oxygen A-band slant path absorption spectrum for a tangent altitude of 20 km. The solid line represents a spectral resolution of ~0.06 nm and the dashed line represents the SAGE III resolution of ~1.4 nm.

3. Temperature and Pressure Retrieval Algorithm

$$\chi^2(\mathbf{T},\mathbf{p}) = \sum_{i=1}^{M}\sum_{j=1}^{N} [A_j^m(\lambda_i) - A_j^c(\lambda_i;\mathbf{T},\mathbf{p})]^2$$

The temperature and pressure dependencies of the oxygen A-band absorption line strengths and widths are second-order effects which are highly non-linear in nature. Accurate retrieval of these parameters requires an inversion technique that will utilize the maximum available spectral information. The technique currently adopted for the SAGE III retrievals is a global fit approach similar to the method described by Carlotti (1988). The global fit method uses a non-linear least squares procedure to simultaneously fit absorption measurements from all spectral channels and slant paths. In this approach, we evaluate a χ^2 merit function and search for a set of temperature and pressure values which minimize it. The χ^2 merit function is defined as

where $A_j^m(\lambda_i)$ are the measured O_2 absorption values (corrected for Rayleigh, aerosol, and ozone) for slant path j and channel i; $A_j^c(\lambda_i;\mathbf{T},\mathbf{p})$ are the computed absorption values for slant path j and channel i as a function of the temperature and pressure; **T** and **p** are vectors of the temperature and pressure profiles from 0 to 85 km; M is the number of tangent heights; and N is the number of channels. The computed absorption values, $A_j^c(\lambda_i;\mathbf{T},\mathbf{p})$, are interpolated from a data base of slant path absorptions generated using line-by-line calculations and the pseudo mass path approximation (Gordley and Russell, 1980).

The global fitting algorithm employs the Marquardt method (Marquardt, 1963) to perform the non-linear least squares fit. The Marquardt method, a well-known procedure that has become a standard of non-linear least-squares routines, minimizes the merit function using an iterative procedure that has the advantage of alternating between the inverse-Hessian method and the steepest descent method as appropriate. Functionally, the retrieval using the Marquardt method will proceed as follows:

(1) the merit function, $\chi^2(\mathbf{T},\mathbf{p})$, will initially be calculated using the first-guess T, p profiles provided by the DAO;

(2) the T, P values are adjusted using either the inverse-Hessian or steepest descent method as appropriate and a new merit function, $\chi^2(\mathbf{T}+\delta\mathbf{T},\mathbf{p}+\delta\mathbf{p})$, is calculated;

(3) the difference between the old and new merit functions, $\chi^2(\mathbf{T},\mathbf{p}) - \chi^2(\mathbf{T}+\delta\mathbf{T},\mathbf{p}+\delta\mathbf{p})$, is calculated;

(4) steps (2)-(3) are repeated until the convergence criteria have been met (typically defined as when the magnitude of $\chi^2(\mathbf{T},\mathbf{p}) - \chi^2(\mathbf{T}+\delta\mathbf{T},\mathbf{p}+\delta\mathbf{p})$ is less than the

estimated uncertainty in the slant path absorption measurements.

We have performed numerous simulated retrievals using this approach. An illustrative example of a temperature retrieval is shown in Figure 2. This retrieval was based on simulated O_2 slant path absorption measurements with realistic random noise (signal-to-noise ratio of 3000). The retrieved values have been smoothed with a 3-km boxcar filter above 40 km. The true atmosphere (dashed line) is based on a radiosonde profile and the "first-guess" profile (dotted line) is derived from NMC gridded analyses. As can be seen, the retrieved profile (solid line) reproduces the true temperature extremely well in the troposphere and lower stratosphere. At higher altitudes, the retrievals tend to oscillate about the true atmosphere. The differences between the "real" and retrieved temperature and pressure profiles at each altitude are shown in Figure 3.

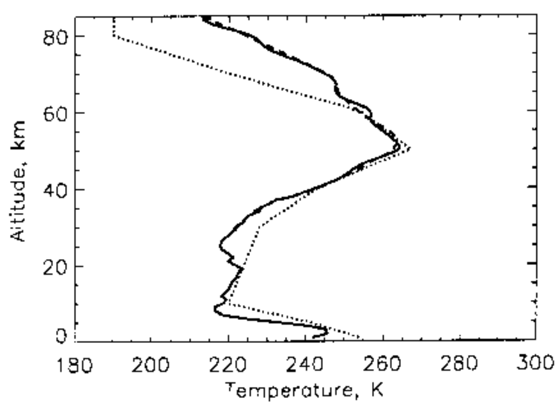

Figure 2. Simulated SAGE III temperature retrieval. The dotted line is the "first-guess" temperature profile, the dashed line is the true atmosphere, and the solid line is the retrieved profile.

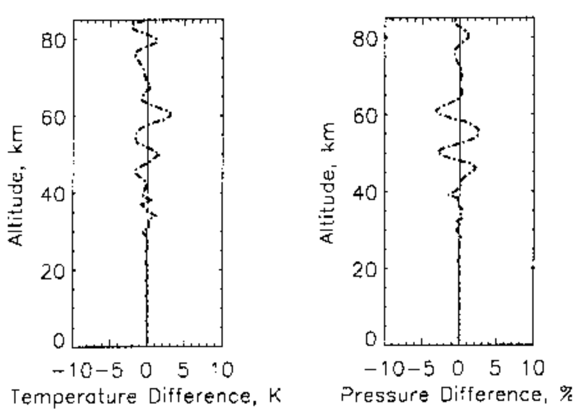

Figure 3. Differences between true and retrieved profiles of temperature and pressure.

4. Uncertainty Estimates

The random component of error in the temperature and pressure retrievals is associated with uncertainties in the residual oxygen A-band slant path absorption values. These uncertainties include both the random noise associated with the SAGE III total A-band slant path absorptivity measurements themselves and the uncertainties involved with removing the Rayleigh scattering, aerosol, and ozone contributions from the A-band measurements. The dominant component will be due to the random noise in the total A-band slant path absorption measurements. In order to estimate the magnitude of this component, we have performed a large number of retrievals with realistic measurement noise and examined the statistical uncertainties. Figure 4 shows the expected uncertainties as a function of height for O_2 A-band measurements with signal-to-noise ratios of 3000. The 1-σ error in the retrieved temperatures range from less than 1°K in the troposphere to approximately 4°K in the mesosphere. The 1-σ error in the retrieved pressures ranges from less than 1% in the troposphere to about 5% in the mesosphere.

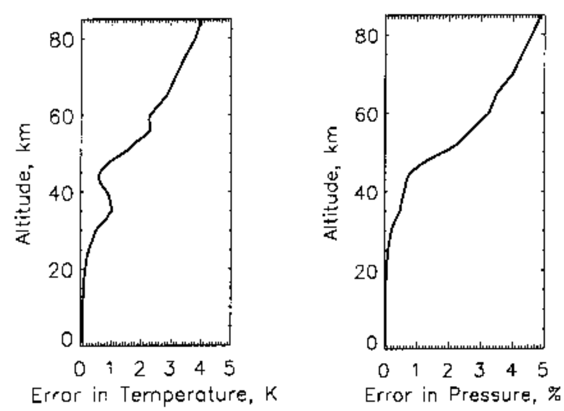

Figure 4. Expected random uncertainties in retrieved temperature and pressure profiles due to measurement noise.

The uncertainties involved with removing the Rayleigh scattering component are due to uncertainties in the "first-guess" temperature profiles obtained from the DAO. These Rayleigh correction uncertainties are estimated from the error bars associated with the DAO profiles and will be independent of altitude. The uncertainties involved with removing the aerosol contribution are expected to be on the order of 1% of the aerosol transmission over the A-band spectral region. The uncertainties involved with removing the ozone contributions are expected to be on the order of 1% of the ozone transmission over the A-band. Although the uncertainties associated with removing the Rayleigh, aerosol, and ozone contributions are random event to event, they may be highly correlated across the A-band spectrum during an individual event. Sensitivity studies are being performed to determine more accurate estimates of these uncertainties. Then, these will be combined with the uncertainties due to measurement noise in an appropriate fashion such as described in Russell et al. (1989) to estimate the total random errors.

In addition to the random uncertainties discussed above, there will be systematic uncertainties associated with the oxygen A-band spectroscopy. Laboratory measurements of the line intensities for the oxygen A-band vary by ~15% while the line widths vary by ~30%. The effect that these line parameter uncertainties will have on the temperature and pressure retrievals will be estimated from sensitivity studies.

5. Future Plans

The retrieval algorithm presented here will be refined as additional test data and simulations become available. A more rigorous characterization and error analysis of the retrievals will be performed using an approach similar to that described by Rodgers (1990). In addition, an excellent opportunity exists to test the SAGE III algorithm with real measurements prior to launch. The Improved Limb Atmospheric Spectrometer (ILAS) is scheduled for launch in August 1996 on the Japanese ADEOS satellite. ILAS is a limb occultation experiment similar to SAGE III and will have 1024 visible channels for measuring atmospheric transmission spectra. ILAS will also perform retrievals of temperature and pressure using oxygen A-band spectra. In cooperation with the ILAS Science Team, we will obtain oxygen A-band transmission measurements and use them as input to the SAGE III retrieval algorithm.

REFERENCES

Carlotti, M., 1988: Global-fit approach to the analysis of limb-scanning atmospheric measurements. *Appl. Opt.*, *27*, 3250-3254.

Gordley, L. L., and J. M. Russell, 1980: A fast and accurate radiance algorithm for applications to inversion of limb measurements. In *Remote Sensing of Atmospheres and Oceans*, edited by A. Deepak, Academic Press, San Diego, Calif., 591-607.

Marquardt, D. W., 1963: An algorithm for least-squares estimation of nonlinear parameters, *J. Soc. Indust. Appl. Math.*, ***11***, 431-441.

Mauldin, L. E., 1984: Stratospheric Aerosol and Gas Experiment II instrument: A functional description, *Opt. Eng.*, **24**, 307-312.

McCormick, M. P., P. Hamill, T. J. Pepin, W. P. Chu, T. J. Swissler, and L. R. McMaster, 1979: Satellite studies of the stratospheric aerosol, *Bull. of the Amer. Met. Soc.*, **60**, 9-12.

McCormick, M. P., W. P. Chu, J. M. Zawodny, L. E. Mauldin, L. R. McMaster, 1991: Stratospheric Aerosol and Gas Experiment III (SAGE III) aerosol and trace gas measurements for Earth Observing System (EOS), SPIE Paper No. 1491-16.

Rodgers, C. D., 1990: Characterization and error analysis of profiles retrieved from remote sounding measurements, *J. Geophys. Res.*, **95**, 5587-5595.

Russell, P. B., T. J. Swissler, M. P. McCormick, W. P. Chu, J. M. Livingston, and T. J. Pepin, 1981: Satellite and correlative measurements of the stratospheric aerosol, I. An optical model for data conversion, *J. Atmos. Sci.*, ***38***, 1279-1294.